

# Exact ground states for coupled spin trimers

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**Abstract.** We consider a class of geometrically frustrated Heisenberg spin systems which admit exact ground states. The systems consist of suitably coupled antiferromagnetic spin trimers with integer spin quantum numbers  $s$  and their ground state  $\Phi$  will be the product state of the local singlet ground states of the trimers. We provide linear equations for the inter-trimer coupling constants which are equivalent to  $\Phi$  being an eigenstate of the corresponding Heisenberg Hamiltonian and sufficient conditions for  $\Phi$  being a ground state. The classical case  $s \rightarrow \infty$  can be completely analyzed. For the quantum case we consider a couple of examples, where the critical values of the inter-trimer couplings are numerically determined. These examples include chains of corner sharing tetrahedra as well as certain spin tubes.  $\Phi$  is proven to be gapped in the case of trimer chains. This follows from a more general theorem on quantum chains with product ground states.

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## 1. Introduction

The effects of frustration in Heisenberg magnets have attracted much interest over the past few decades [1, 2]. Geometrically frustrated quantum antiferromagnets (AF) are an excellent play-ground for studying novel quantum many-body phenomena. We mention quantum spin-liquid phases, valence-bond crystal phases, order-by-disorder phenomena, lattice instabilities to name just a few.

Moreover, in recent years there has been remarkable progress in synthesizing magnetic materials [3]. Even exotic structures such as the star [4] or the maple-leaf lattices [5] have been synthesized. Hence, the investigation of exotic lattice structures being on the first glance purely academic might become relevant for experimental studies.

The theoretical investigation of frustration effects in quantum spin antiferromagnets usually meets new difficulties; e. g. the quantum Monte Carlo method suffers from the sign problem for frustrated systems. Exact statements for interacting quantum-many body systems are rare and, therefore, new rigorous results are of considerable interest to improve their understanding. Moreover, solvable models may serve as test grounds for approximate methods.

Starting with the seminal papers of Majumdar-Ghosh [6] and Shastry-Sutherland [7], a famous class of spin systems with exact ground states has thoroughly been investigated, see, for example, [8]. These systems consist of  $N$  suitably coupled AF dimers such that the product state of the local  $S = 0$  dimer ground states remains the ground state of the total system. For this it is necessary that the coupling constants between the dimers satisfy certain linear equations [9]. A generalization to chains with trimerized ground states using  $SU(3)$  spins and bilinear-biquadratic Hamiltonians has recently been published [10]. Another approach using matrix product states as exact ground states [11] has also been mainly applied to anisotropic spin systems.

In this paper we will rather consider isotropic (Heisenberg) spin systems and extend the basic idea underlying the Majumdar-Ghosh-Shastry-Sutherland ground states to systems with AF trimers as building blocks. These systems will be geometrically frustrated. If the individual spin quantum number  $s$  is integer, the ground state of a uniform (or almost uniform) AF trimer will be again a non-degenerate singlet state, i. e. having  $S = 0$ . The product state  $\Phi$  of these local ground states will be an eigenstate of the Heisenberg Hamiltonian of  $N$  trimers if and only if the coupling constants satisfy certain linear constraints completely analogous to the dimer case. Moreover, if the coupling between the dimers is not too strong,  $\Phi$  will be the ground state of the total system, called the *trimerized ground state* (TGS). Of course, the question arises what precisely is meant by "not too strong"? In general, the precise domain of systems admitting TGS can only be numerically investigated for given examples and lattice structures. In a

sense, we thus invert the usual strategy to numerically find ground states for given spin systems. We define a certain state  $\Phi$  and numerically calculate the coupling constants for systems which have  $\Phi$  as their ground state. However, we have also derived some general rigorous statements on systems with trimerized ground states. These statements mainly concern trimerized ground states in the classical limit  $s \rightarrow \infty$ , which can be completely understood, and some sufficient conditions for trimerized ground states in the quantum case. Moreover, we prove that in the case of trimer chains with trimerized ground state,  $\Phi$  will be gapped for an extended domain of coupling constants. We stress that our investigation is restricted to the case of integer  $s$ , since for  $s$  being half integer the ground state of the AF trimer will be degenerate, see, e. g. [12]. We mention that trimerized states of the kind explained above have also been considered as approximate ground states of certain modified 2D kagome lattices [13].

The paper is organized as follows. In section 2 we summarize the basic definitions and main results. Section 3 is devoted to a couple of examples, starting from a single trimer, followed by a pair of trimers and then passing to 1-dimensional chains of trimers. The latter examples cover systems like chains of corner-sharing tetrahedra [14] and spin tubes [15], which currently attract a lot of attention in the literature, albeit, as a rule, not under the aspect of exact ground states. The study of the examples led us to some conjectures about the domain of the coupling constants for systems admitting trimerized ground states and its dependence on  $s$  and  $N$ . In order to clearly distinguish these conjectures from the mentioned rigorous statements we have presented the latter in a separate section 4. We decided to give detailed proofs of these statements only in those cases where they markedly differ from the analogous proofs for the dimer case in [9].

## 2. Basic definitions and summary of main results

We consider systems of  $3N$  spins with one and the same individual integer spin quantum number  $s = 1, 2, 3, \dots$  which are grouped into  $N$  fixed triples (“trimers”). To indicate this grouping the spins will be denoted by indices  $\mu = (i, \delta)$  where  $i = 1, \dots, N$  is the trimer index and  $\delta = 0, 1, 2$  distinguishes between the three spins belonging to the same trimer. Further we consider Heisenberg Hamiltonians

$$\tilde{H}(\mathbb{J}) = \sum_{\mu\nu} J_{\mu\nu} \tilde{\mathbf{s}}_{\mu} \cdot \tilde{\mathbf{s}}_{\nu} \quad (1)$$

$$= \sum_{i,j} \sum_{\delta,\epsilon} J_{i\delta,j\epsilon} \tilde{\mathbf{s}}_{i\delta} \cdot \tilde{\mathbf{s}}_{j\epsilon} , \quad (2)$$

where  $\tilde{\mathbf{s}}_{\mu} = (s_{\mu}^{(1)}, s_{\mu}^{(2)}, s_{\mu}^{(3)})$  denotes the  $\mu$ -th spin observable and  $\mathbb{J}$  the  $3N \times 3N$ -matrix of real exchange parameters or coupling constants  $J_{\mu\nu}$  satisfying

$$J_{\mu\mu} = 0, \quad J_{\mu\nu} = J_{\nu\mu} \text{ for all } \mu, \nu = 1, \dots, 3N . \quad (3)$$

All operators act on a  $(2s+1)^{3N}$ -dimensional Hilbert space  $\mathcal{H} = \bigotimes_{\mu=1}^{3N} \mathcal{H}_\mu$ . If the spin quantum number  $s$  is fixed, we may identify a spin system with its matrix  $\mathbb{J}$ . Note that due to the matrix notation each scalar product  $\mathbf{s}_\mu \cdot \mathbf{s}_\nu$  occurs twice in the Hamiltonian (1). In order to comply with the usual notation we have therefore introduced the factor  $\frac{1}{2}$  in some examples of section 3.

For any trimer with index  $i$  let  $[i0, i1, i2]$  denote the ground state of the AF trimer  $\tilde{H}_0 = \lambda_i \sum_{\delta, \epsilon} \mathbf{s}_{i\delta} \cdot \mathbf{s}_{i\epsilon}$ ,  $\lambda_i > 0$  which is unique up to a phase factor. If the trimer index  $i$  is irrelevant, it will be simply denoted by  $[0, 1, 2]$ . For general  $s$  this state can be written in terms of the Wigner-3j-symbol as

$$[0, 1, 2] = \sum_{m_0, m_1 = -s}^s \begin{pmatrix} s & s & s \\ m_0 & m_1 & -m_0 - m_1 \end{pmatrix} |m_0, m_1, -m_0 - m_1\rangle, \quad (4)$$

using the eigenbasis  $|m\rangle$ ,  $m = -s, \dots, s$  of  $\mathbf{s}_\mu^{(3)}$  and the corresponding product bases. The state  $[i0, i1, i2]$  will remain the ground state of the trimer  $i$  even when its Hamiltonian is suitably disturbed, see section 3.1. Let  $\mathcal{C}_i^s$  denote the set of all  $(J_{i0}, J_{i1}, J_{i2})$  where this is the case.

The ground state of a system of  $N$  unconnected AF trimers satisfying  $(J_{i0}, J_{i1}, J_{i2}) \in \mathcal{C}_i^s$  for  $i = 1, \dots, N$  is the product state

$$\Phi^s \equiv \bigotimes_{i=1}^N [i0, i1, i2], \quad (5)$$

called the *trimerized state*; it has the total spin quantum number  $S = 0$ . A system  $\mathbb{J}$  is said to admit trimerized ground states (TGS), or to have the TGS property, iff  $\Phi^s$  is a ground state of  $\tilde{H}(\mathbb{J})$ , i. e. iff

$$\langle \Phi^s | \tilde{H}(\mathbb{J}) | \Phi^s \rangle \leq \langle \Psi | \tilde{H}(\mathbb{J}) | \Psi \rangle \quad (6)$$

for all  $\Psi \in \mathcal{H}$  with  $\|\Psi\| = 1$ . Let  $\mathcal{C}_\Phi^s$  denote the set of all spin systems  $\mathbb{J}$  with the TGS property. If the quantum number  $s$  is understood, we suppress it and write simply  $\Phi$  and  $\mathcal{C}_\Phi$ .

For  $\mathbb{J} \in \mathcal{C}_\Phi$  it is necessary that  $\Phi$  will be an eigenstate of  $\tilde{H}(\mathbb{J})$ . This turns out to be true if and only if the inter-trimer coupling constants fulfil the relations

$$J_{i0,j0} + J_{i1,j1} = J_{i0,j1} + J_{i1,j0} \quad (7)$$

$$J_{i0,j0} + J_{i1,j2} = J_{i0,j2} + J_{i1,j0} \quad (8)$$

$$J_{i0,j0} + J_{i2,j1} = J_{i0,j1} + J_{i2,j0} \quad (9)$$

$$J_{i0,j0} + J_{i2,j2} = J_{i0,j2} + J_{i2,j0} \quad (10)$$

for all  $1 \leq i < j \leq N$ . The corresponding eigenvalue

$$E = -s(s+1) \left( \sum_{i=1}^N J_{i0,i1} + J_{i0,i2} + J_{i1,i2} \right). \quad (11)$$

is independent of the inter-trimer coupling. Since (7)-(10) is a system of four independent linear equations, the set of all real, symmetric  $3N \times 3N$ -matrices satisfying (7)-(10) and  $J_{\mu\mu} = 0$  for all  $\mu = 1, \dots, 3N$  will be a linear space of dimension  $3N + 5\binom{N}{2} = \frac{N}{2}(5N+1)$ , denoted by  $\mathcal{J}_\Phi$ . The set  $\mathcal{C}_\Phi$  of TGS systems will form a convex cone embedded in the linear space  $\mathcal{J}_\Phi$ , since the condition (6) is invariant under positive linear combinations of  $\mathbb{J}$ 's, see also [9]. At the boundary of  $\mathcal{C}_\Phi$ , the trimerized ground state  $\Phi$  will become degenerate, i. e. there will exist “competing” ground states which have a lower energy than (11) if  $\mathbb{J}$  crosses the boundary of  $\mathcal{C}_\Phi$ . Sometimes we will also use the symbol  $\overset{\circ}{\mathcal{C}}_\Phi$  in order to denote the open convex cone of spin systems  $\mathbb{J}$  where  $\Phi$  is a non-degenerate ground state.

The conditions (7)-(10) still include interesting spin structures such as corner-sharing tetrahedra and spin tubes to be considered in section 3.3. In some of these chains additional symmetries arise which allow the description by an equivalent ladder model of composite spins, see 3.3.1 and 3.3.2. However, the TGS property is independent of this additional symmetry as shown by the example of a certain spin tube in section 3.3.2.

It is clear that the choice of dimensionless numbers for the  $J_{\mu\nu}$  in the examples implies the introduction of appropriate units for energy and temperature in order to apply the Heisenberg model to real systems. In this sense, temperature becomes a dimensionless quantity in the thermodynamic calculations of section 3.2 which illustrate some physical consequences of the existence of TGS ground states. In most cases the domain of TGS systems, i. e. the shape of the cone  $\mathcal{C}_\Phi^s$  can only be determined numerically. Exceptions are the single trimer case where  $\mathcal{C}_\Phi^s$  can be calculated analytically, see section 3.1, and the two-trimer case with  $s = 1$ , see section 3.2. In all examples which are considered in section 3 there is some evidence that these cones shrink with increasing  $s$ . Note that in the classical limit  $\mathcal{C}_\Phi^\infty$  will be degenerate, since the necessary conditions for the  $J_{\mu\nu}$  are stronger in this case, see section 4.2. In contrast, for the chains of trimers considered in section 3.3, the dependence of  $\mathcal{C}_\Phi^s$  on  $N$  is only weak. Moreover, we found that  $\mathcal{C}_\Phi^s$  is slightly expanding if  $N$  grows. This is an indication that the limit of  $\mathcal{C}_\Phi^s$  for  $N \rightarrow \infty$  is “non-degenerate”, in the sense that it does not converge to a lower-dimensional domain and that the trimerized ground state is gapped. We will rigorously prove these properties in section 4.4. Our class of models thus supports Haldane’s conjecture [16] that integer spin chains possess a unique ground state and an energy gap between the ground state and the excited states. The famous AKLT model [17] is also an  $s = 1$  spin chain with a unique gapped ground state but its anti-ferromagnetic Heisenberg Hamiltonian is modified by a biquadratic term. For the  $s = 1/2$  Heisenberg spin chain the absence of an energy gap has been proven in the ‘Lieb-Schultz-Mattis theorem’ [18].

In the classical case  $s \rightarrow \infty$  an analogous definition of TGS systems is possible, see section 4. In this case  $\Phi$  consists of all spin configurations with a mutual angle of  $120^\circ$  between spin vectors of the same trimer. For classical TGS systems the inter-trimer coupling must be necessarily uniform and hence can be described by a symmetric  $N \times N$ -matrix  $\mathbb{G}$ . We have the result that a classical system has the TGS property if and only if  $\mathbb{G}$  is positive semi-definite. Thus the classical case is completely understood.

### 3. Examples

For readers less interested in the mathematical details of our rigorous analysis that will be presented in more detail below in section 4 we first present some examples. In particular, the general statements listed above can be used to discuss certain specific chain-like models, such as chains of corner sharing tetrahedra as well as various spin tubes. We begin with some more elementary examples.

#### 3.1. One Trimer

We consider three spins with integer spin quantum number  $s$  and Heisenberg Hamiltonian

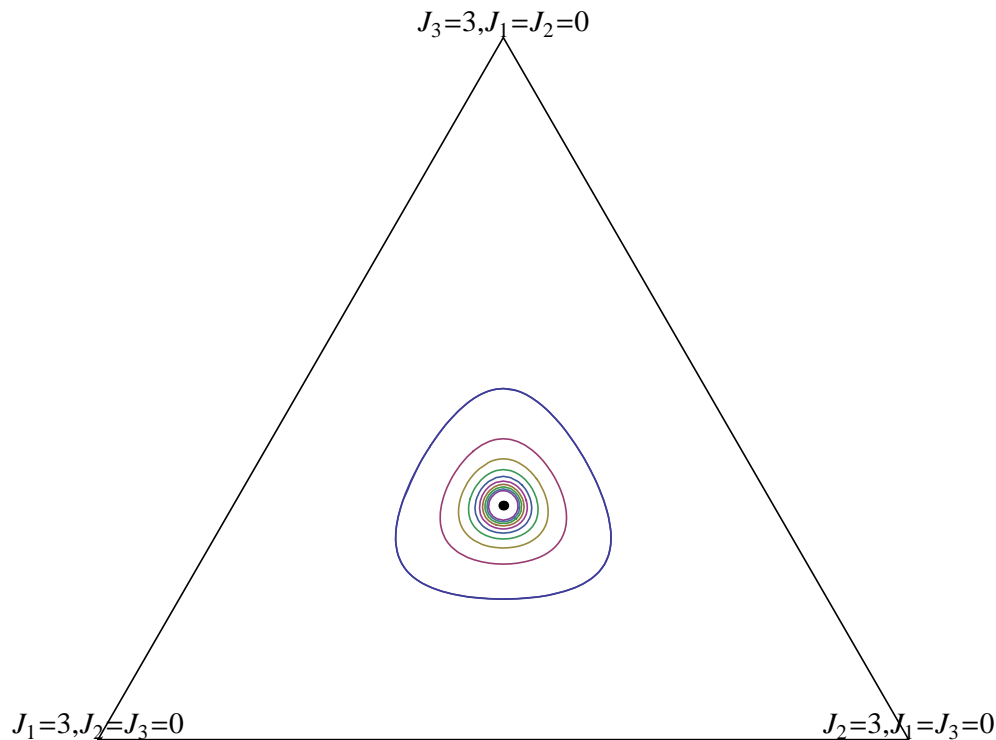
$$\tilde{H} = \sum_{\mu, \nu=1}^3 J_{\mu\nu} \mathbf{s}_\mu \cdot \mathbf{s}_\nu = J_1 \mathbf{s}_2 \cdot \mathbf{s}_3 + J_2 \mathbf{s}_3 \cdot \mathbf{s}_1 + J_3 \mathbf{s}_1 \cdot \mathbf{s}_2, \quad (12)$$

where we have relabeled the coupling constants in order to keep the following formulas readable. Let  $[1, 2, 3]$  denote the unique state with vanishing total spin,  $S = 0$ . It is an eigenstate of (12), since the eigenspaces of  $\tilde{S}^2$  are invariant under  $\tilde{H}$ . For certain values of  $J_1, J_2, J_3$ ,  $[1, 2, 3]$  is even the ground state of  $\tilde{H}$ , e. g. for  $J_1 = J_2 = J_3 = 1$ . These values of  $J_1, J_2, J_3$  form an closed convex cone  $\mathcal{C}^s$  in the 3-dimensional  $(J_1, J_2, J_3)$ -space. At the boundary of  $\mathcal{C}^s$  the ground state of  $\tilde{H}$  becomes degenerate. Recall that  $\overset{\circ}{\mathcal{C}}^s$  denotes the open subset of  $\mathcal{C}^s$  where  $[1, 2, 3]$  is the non-degenerate ground state. The form of the cone can be calculated using computer-algebraic software and the well-established assumption that the competing state has the quantum number  $S = 1$ . It is given by the following inequalities

$$\begin{aligned} (J_1, J_2, J_3) \in \overset{\circ}{\mathcal{C}}^s & \Leftrightarrow \\ \frac{1}{2}s(s+1)(J_1 + J_2 + J_3)(J_1 J_2 + J_2 J_3 + J_3 J_1) & < (1 + \frac{9}{2}s(s+1))J_1 J_2 J_3 \\ \text{and } J_1, J_2, J_3 > 0. & \end{aligned} \quad (13)$$

The intersection of  $\mathcal{C}^s$ ,  $s = 1, \dots, 10$  with the plane  $J_1 + J_2 + J_3 = 3$  is depicted in figure 1. By Taylor expansion of (13) one can show that, for increasing values of  $s$ , the cones  $\mathcal{C}^s$  approach a circular form centered at the half line  $J_1 = J_2 = J_3 > 0$  with a cone angle of

$$\vartheta = \arctan \sqrt{\frac{2}{3(1 + 3s(s+1))}}. \quad (14)$$



**Figure 1.** Representation of the neighborhood of  $J_1 = J_2 = J_3 = 1$  in which the state  $[1, 2, 3]$  remains the ground state of (12) where  $s = 1, \dots, 10$  starting with the outermost curve. The values of  $J_1, J_2, J_3$  are restricted to the plane  $J_1 + J_2 + J_3 = 3$ . The curves have been calculated according to (13) and have been confirmed numerically for  $s = 1, \dots, 5$ . The point at the center of the figure with coordinates  $(1, 1, 1)$  corresponds to the classical limit.

Hence the cones  $\mathcal{C}^s$  will shrink and approach their classical limit  $J_1 = J_2 = J_3 > 0$  for  $s \rightarrow \infty$ , see section 4.

### 3.2. Two Trimers

Next we consider two trimers, i. e. six spins grouped into two triples with indices  $(1, 2, 3)$  and  $(4, 5, 6)$  and Heisenberg Hamiltonian

$$\tilde{H} = \sum_{\mu, \nu=1}^6 J_{\mu\nu} \tilde{\mathbf{s}}_{\mu} \cdot \tilde{\mathbf{s}}_{\nu} . \quad (15)$$

We ask whether  $\Phi \equiv [1, 2, 3] \otimes [4, 5, 6]$  will be a ground state of  $\tilde{H}$ .  $\Phi$  is then called the *trimerized ground state*. First, we note that  $\Phi$  need not be an eigenstate of  $\tilde{H}$  unless the  $J_{\mu\nu}$  do not satisfy equations (7)-(10). These equations will be derived in section 4. They can be expressed in the following way: Let  $(X, Y)$  be a pair of spins belonging to the first trimer and  $(x, y)$  another pair belonging to the second one. Then the two sums  $J_{Xx} + J_{Yy}$  and  $J_{Xy} + J_{Yx}$  must be equal. This is a kind of balance condition completely analogous to the corresponding condition in the case of two dimers, see [9]. It is satisfied

for all combinations of spin pairs if and only if  $\Phi$  is an eigenstate of  $H$ . Actually, only four conditions of the above form have to be postulated, since the other will follow then, see section 4. The coupling constants within the same trimer are not constrained, hence we are left with a  $3 + 3 + 5 = 11$ -dimensional linear space of independent coupling constants  $J_{\mu\nu}$ , which will be called  $\mathcal{J}$ . It is independent of  $s$ .

Again, the linear space  $\mathcal{J}$  will contain a closed convex cone  $\mathcal{C}^s$  of values  $J_{\mu\nu}$  such that  $\Phi$  will be a ground state of the corresponding Hamiltonian (15). The example of two unconnected trimers with the respective non-degenerate ground states  $[1, 2, 3]$  and  $[4, 5, 6]$  shows that  $\mathcal{C}^s$  is not empty. But it seems hopeless to analytically calculate  $\mathcal{C}^s$  except for  $s = 1$ . Thus we will here present some mixture of numerical, computer-algebraic and semi-analytical results. Neglecting a positive overall factor in (15) we still have a 10-dimensional manifold of possible  $J_{\mu\nu}$ -values which is difficult to visualize. We will hence confine ourselves to some two-dimensional subspace of  $\mathcal{J}$  defined by (see also figure 2)

$$J_{12} = J_{13} = J_{23} = J_{45} = J_{46} = J_{56} = \frac{1}{2} \text{ and} \quad (16)$$

$$J_{14} = -J_{26} = -J_{36} = \frac{a}{2}, \quad J_{15} = \frac{b}{2}, \quad J_{25} = J_{35} = \frac{b-a}{2}, \quad (17)$$

where obviously the second equation fulfils the general conditions (7)-(10). Note that the coupling strength between spins indicated in figure 2 equals twice the values of the  $J_{\mu\nu}$  due to our definition of the Hamiltonian (15).

The set  $\mathcal{T}^s$  of points with coordinates  $(a, b)$  such that  $\Phi$  will be a ground state of the corresponding Hamiltonian is again a convex set. It is represented in figure 5 for the values  $s = 1, 2, 3, 4, 5$ . The case  $s = 1$  is just within the practical limits of computer-algebraic methods. The boundary of  $\mathcal{T}^1$  consists of pieces of 6 intersecting curves given by equations of the form  $q_{ij}(a, b) = 0$  where the  $q_{ij}$  are polynomials in the variables  $a, b$  with integer coefficients. The three simplest cases are

$$q_{00} = 4 - 4a - a^2 + a^3 - 4b + 5ab - a^2b - b^2 - ab^2 + b^3, \quad (18)$$

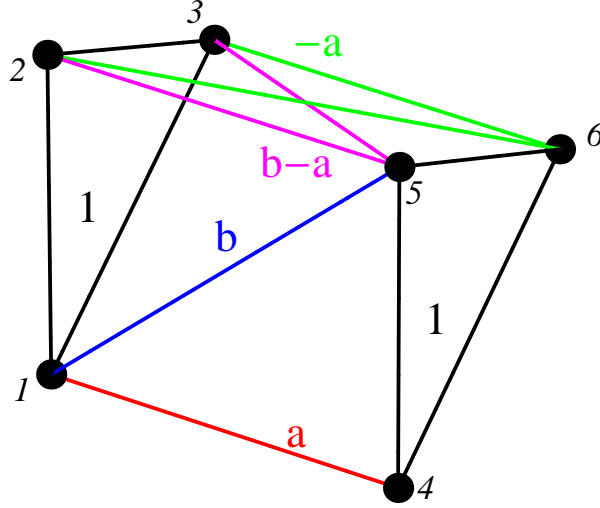
$$q_{02} = 8 + 28a + 28a^2 + 8a^3 - 8b - 14ab - 5a^2b - 2b^2 - 5ab^2 + 2b^3, \quad (19)$$

and

$$\begin{aligned} q_{10} = & 128 - 128a - 74a^2 + 85a^3 - 2a^4 - 11a^5 + 2a^6 - 128b + 226ab - 29a^2b \\ & - 68a^3b + 25a^4b - 2a^5b - 74b^2 - 29ab^2 + 66a^2b^2 - 8a^3b^2 - 2a^4b^2 + 85b^3 \\ & - 68ab^3 - 8a^2b^3 + 4a^3b^3 - 2b^4 + 25ab^4 - 2a^2b^4 - 11b^5 - 2ab^5 + 2b^6. \end{aligned} \quad (20)$$

The other polynomials are too complicated to be reproduced here. Note that the Hamiltonian (15) with the coupling constants (16, 17) commutes with  $\mathcal{S}^2$  and  $\mathcal{S}_{23}^2$ . Correspondingly, the indices  $i, j$  of the polynomials  $q_{ij}$  refer to the quantum numbers  $S \equiv i$  and



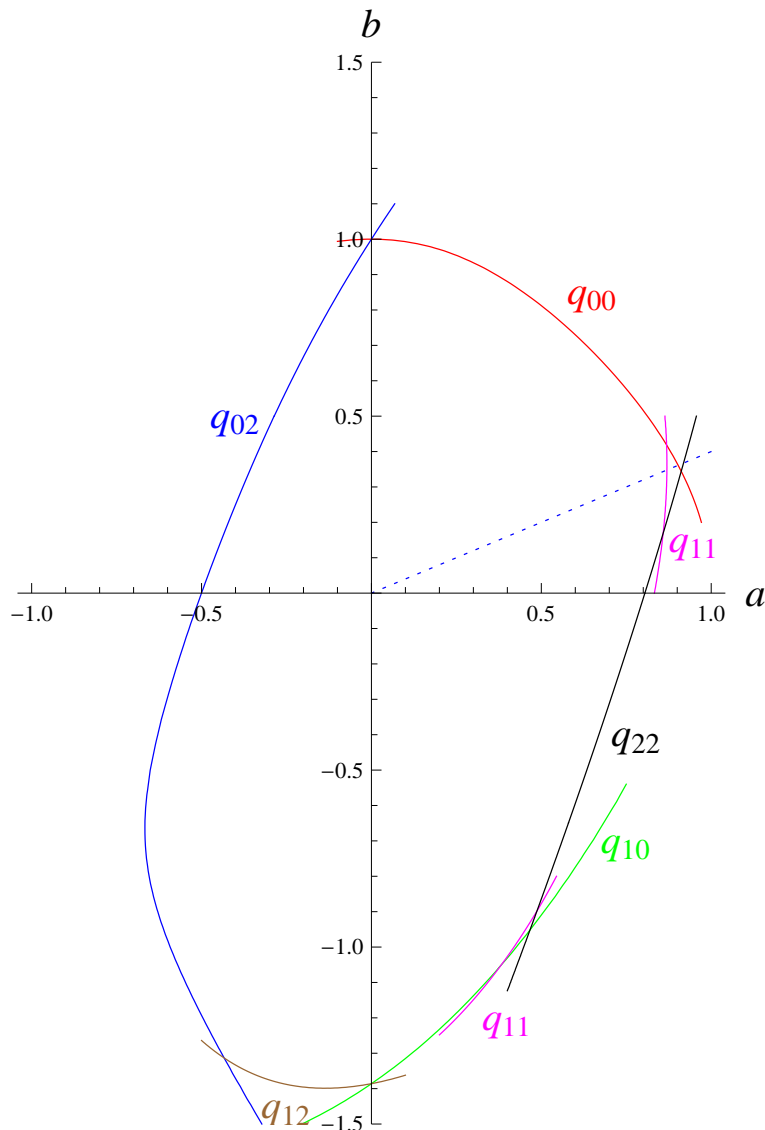


**Figure 2.** Two coupled trimers satisfying (16),(17). The intra-trimer coupling (black lines) is set to one. The inter trimer coupling strengths are  $a$  (red line),  $-a$  (green line),  $b$  (blue line) and  $b - a$  (magenta line).

$S_{23} \equiv j$  of the corresponding competing states, see figure 3.

In order to illustrate the physical implications of the presence of TGS ground states for a relatively simple example we have calculated the (dimensionless) zero-field magnetic susceptibility  $\chi = \langle \frac{\partial M}{\partial B} \rangle \big|_{B=0} = \frac{1}{T} \langle M^2 \rangle$  as a function of temperature  $T$  for coupling constants along the line  $b = 0.4a$  and  $s = 1$ , see figure 4. This line crosses the boundary of the TGS domain  $\mathcal{T}^1$  at the value  $a_1 = 0.869506904299778$ . For  $a < a_1$  the ground state  $\Phi$  has  $S = 0$ ; for  $a > a_1$  the competing ground states have  $S = 1$ . Hence there is a transition from  $\chi(T)$  vanishing exponentially at  $T = 0$  to divergence of the form  $\chi(T) \sim \frac{2}{3} \frac{1}{T}$ . The factor  $\frac{2}{3}$  is simply the mean value of  $M^2$  for the three ground states with  $S = 1$  and  $M = -1, 0, 1$ . For  $a = a_1$  the factor is  $\frac{1}{2}$ , corresponding to the mean value of  $M^2$  for the four ground states with  $S = 1$  and  $M = -1, 0, 1$  and  $S = M = 0$ . This transition is qualitatively the same for gapped infinite TGS chains, see section 4.4, although the factor  $\frac{2}{3}$  would have to be replaced by the mean value of  $M^2$  of a continuum of competing ground states.

In the two-trimer example the sets  $\mathcal{T}^s$  are shrinking when  $s$  increases. We generally conjecture that  $\mathcal{C}^s \supset \mathcal{C}^{s'}$  for  $s < s'$  but could not prove this rigorously. For  $b = 0$  and

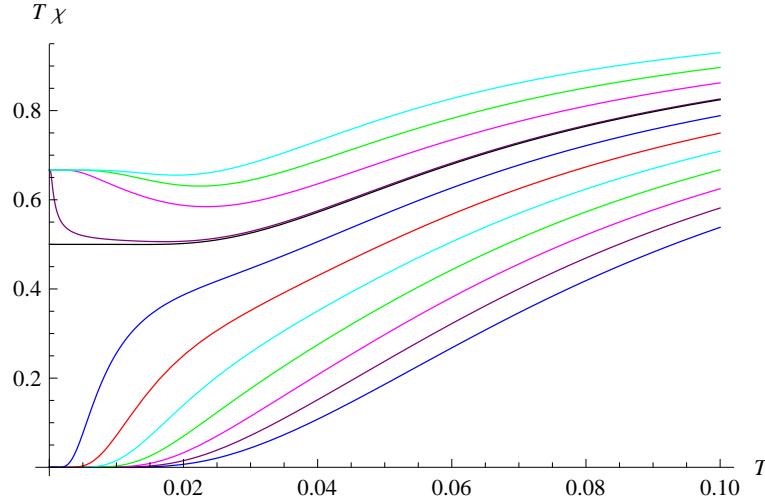


**Figure 3.** Representation of the set  $\mathcal{T}^s$ ,  $s = 1$ , of points with coordinates  $(a, b)$  such that the singlet product state  $\Phi$  will be a ground state of the Hamiltonian (15) corresponding to (16,17). The boundary of  $\mathcal{T}^1$  consists of pieces of 6 intersecting smooth curves  $q_{ij}$  which have been calculated by computer-algebraic means. Note that  $q_{11}$  contributes twice to the boundary. The indices  $i, j$  of  $q_{ij}$  refer to the quantum numbers  $S \equiv i$  and  $S_{23} \equiv j$  of the corresponding competing states. The dotted line defined by  $b = 0.4a$  will be used for thermodynamic calculations, see figure 4.

$a < 0$  we find numerically that the critical value  $a_{\text{crit}}$  which lies at the boundary of  $\mathcal{T}^s$  has the form

$$a_{\text{crit}} = -\frac{1}{s+1} \text{ for } s = 1, 2, 3, 4, 5. \quad (21)$$

This can be confirmed semi-analytically to hold for all  $s$  by calculating the competing state  $\Psi$  which becomes an additional ground state if  $a$  assumes the value  $a_{\text{crit}}$ . We defer this calculation to the Appendix.



**Figure 4.** The product of temperature  $T$  and zero-field susceptibility  $\chi$  as a function of  $T$  for the coupling constants in (17) varying from  $a = 0.8$  (lowermost curve) to  $a = 0.9$  (uppermost curve) and  $b = 0.4a$ . The units are chosen such that  $T\chi = \langle M^2 \rangle$  becomes dimensionless. At the value  $a_1 = 0.869506904299778$  (black curve) the line  $b = 0.4a$  crosses the boundary of the TGS domain and consequently there is a transition from 0 to the finite value  $1/2$  resp.  $2/3$  of  $\lim_{T \rightarrow 0} T\chi$  due to the finite magnetization of the competing state with  $S = 1$ , see figure 3.

### 3.3. Chains

Next we consider examples of chains formed of trimers which are coupled in a balanced way, i. e. satisfying (7)-(10), such that the singlet product state

$$\Phi = \bigotimes_{i=1}^N [i0, i1, i2] \quad (22)$$

becomes an eigenstate of the corresponding Hamiltonian. The coupling within the trimers is always chosen as

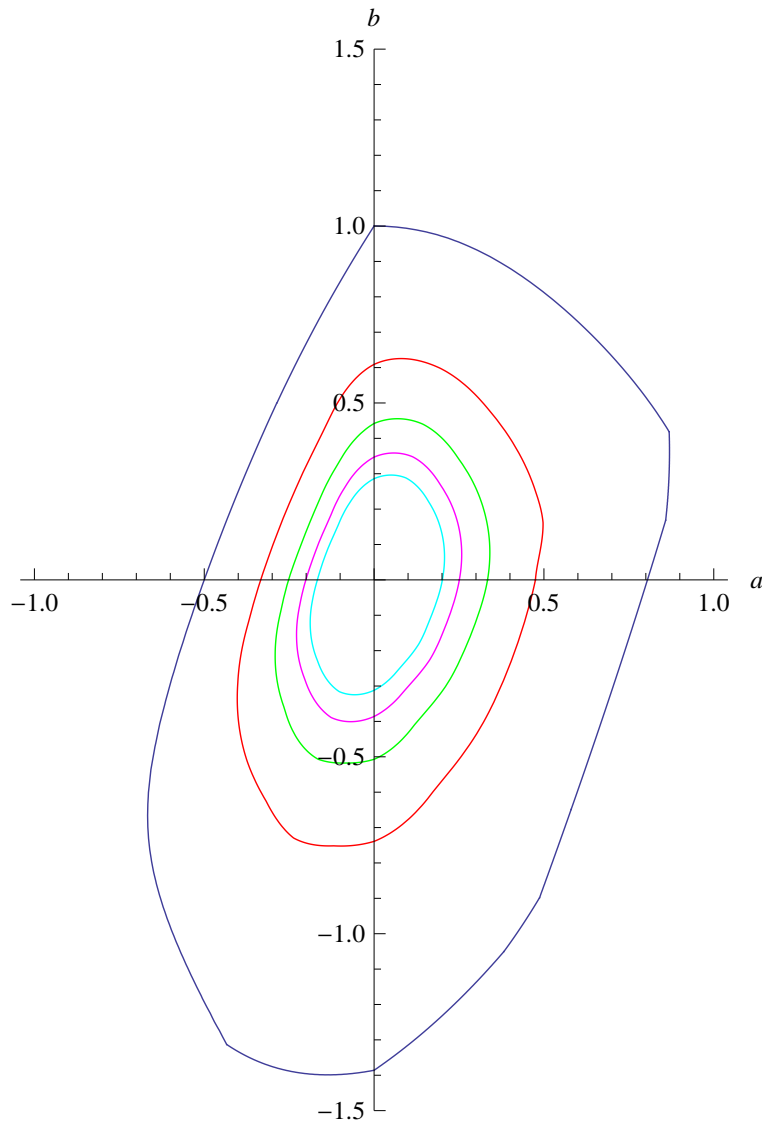
$$J_{i0,i1} = J_{i1,i0} = J_{i0,i2} = J_{i2,i0} = J_{i1,i2} = J_{i2,i1} = \frac{1}{2}. \quad (23)$$

The coupling constants between the trimers  $J_{\delta,\epsilon} \equiv J_{i\delta,(i+1)\epsilon}$  are chosen to depend linearly on one or two parameters and we will investigate the convex domain of these parameters for which  $\Phi$  will be a ground state of the corresponding Hamiltonian. Throughout this section we adopt periodic boundary conditions, i. e.  $N + 1 \equiv 1$ .

#### 3.3.1. Chains of corner sharing tetrahedra

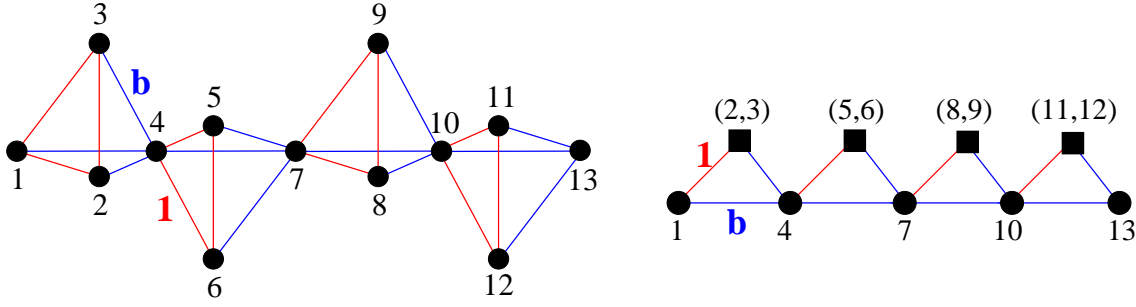
The choice of the inter-trimer interaction matrix

$$(J_{\delta,\epsilon}) = \frac{1}{2} \begin{pmatrix} b & 0 & 0 \\ b & 0 & 0 \\ b & 0 & 0 \end{pmatrix} \quad (24)$$



**Figure 5.** Representation of the set  $\mathcal{T}^s$  of points with coordinates  $(a, b)$  such that the singlet product state  $\Phi$  will be a ground state of the Hamiltonian (15) corresponding to (16,17). The different curves defining the boundary of  $\mathcal{T}^s$  refer to the values of  $s = 1, 2, 3, 4, 5$  starting from the outermost curve. The curve for  $s = 1$  has been calculated analytically, see figure 3, the other curves for  $s = 2, 3, 4, 5$  have been determined numerically.

leads to a chain of corner sharing tetrahedra, see figure 6. Similar systems have been widely considered theoretically as well as experimentally, see e. g. [14]. However, most of these studies are focussed on spin-half systems. As it is typical for chains of corner sharing tetrahedra the chains considered in this section have an additional symmetry, namely that certain composite spin squares (in figure 6 these are  $\tilde{S}_{23}^2$ ,  $\tilde{S}_{56}^2$ , etc. ) commute with the Hamiltonian. Hence we have a simpler sawtooth chain composed of spins and composite spins, see figure 6. While in general the composite spins may have spin quantum number  $s_{\text{comp}} = 0, \dots, 2s$ , in the singlet product ground state  $\Phi$  the composite



**Figure 6.** Example of a chain consisting of corner sharing tetrahedra (left) and an equivalent effective chain of composite spins (right).

spins have the same spin quantum number  $s$  as the individual spins.

We have numerically determined the critical values  $b_{\min}$  and  $b_{\max}$  where  $\Phi$  ceases to be the unique ground state with energy  $E_0 = -\frac{3N}{2}s(s+1)$ . These critical values depend on the number of spins  $3N$  and the spin quantum number  $s$ . The results are contained in table 1. While the dependence on the length of the chain is weak, again an increase in the spin quantum number leads to a significant smaller parameter region where  $\Phi$  is the ground state. From the numerical data we can detect the competing states which become ground states for  $b < b_{\min}$  and  $b > b_{\max}$ . The competing state for negative, i.e. ferromagnetic,  $b$  is a ferrimagnetic state (the total spin of the chain  $S$  is finite but less than  $3Ns$ ) and the composite spins have the spin quantum number  $s-1$ . Hence for  $s=1$  the spin quantum number of the composite spins in the competing state is zero. Then the spins along the base line of the effective sawtooth chain build a simple ferromagnetic  $s=1$  chain which is decoupled from the composite spins. The energy of the competing state is  $\tilde{E}_0 = N(-2+b)$  and its total spin is  $S=N$ . As a result there is a prominent transition for  $s=1$  at  $b_{\min} = -1$ . For  $s > 1$  and ferromagnetic  $b$  there is no simple competing state, since the effective chain is a mixed-spin sawtooth chain [19] (e.g. a mixed spin-one spin-two sawtooth chain in case of  $s=2$ ).

The competing state for positive, i.e. antiferromagnetic,  $b$  is a state with the total spin of the chain  $S=0$  and the composite spins have the spin quantum number  $s-1$ . Again for  $s=1$  the spin quantum number of the composite spins in the competing state is zero, and, as a result, the spins along the base line of the sawtooth build an antiferromagnetic  $s=1$  Haldane chain which is decoupled from the composite spins. The energy of the competing state is  $E'_0 = N(-2 + be_0(N))$ . Setting  $E'_0 = E_0$  yields  $b_{\max} = -\frac{1}{e_0(N)}$ . For  $N \rightarrow \infty$  the energy of the antiferromagnetic chain is given by  $e_0(\infty, 1) = -1.40148403897$ , see [20]. Hence we get for  $N \rightarrow \infty$  the critical value  $b_{\max} = -1/e_0(\infty, 1) = 0.713529353$ . This result together with  $b_{\min} = -1$  indicates that the domain of TGS systems slightly expands with growing  $N$ . Hence we expect a non-degenerate TGS domain even for  $N \rightarrow \infty$  where  $\Phi$  will be a gapped ground state as we will prove in section 4.4. For  $s > 1$  the effective chain is again a mixed-spin sawtooth

**Table 1.** Critical values of the coupling constant  $b$  corresponding to the chains of figure 6.

$3N$	$s$	$b_{\min}$	$b_{\max}$
12	1	-1.0	0.667
12	2	-0.57	0.434
18	1	-1.0	0.696
24	1	-1.0	0.706
30	1	-1.0	0.710

chain and one can find values for  $b_{\max}$  for short chains only.

Finally, we have numerically calculated the energy gap  $\Delta_N$  of the chain of  $N$  corner sharing tetrahedra as a function of the coupling constant  $b$  for  $N = 2, 3, 4, 5$ , see figure 7. These results confirm the rigorous bound  $\Delta_N \geq \Delta_2$  for all  $N = 3, 4, \dots$ , which will be derived in section 4.4, corollary 2 and shows that the TGS ground state is gapped for trimer chains of this kind.

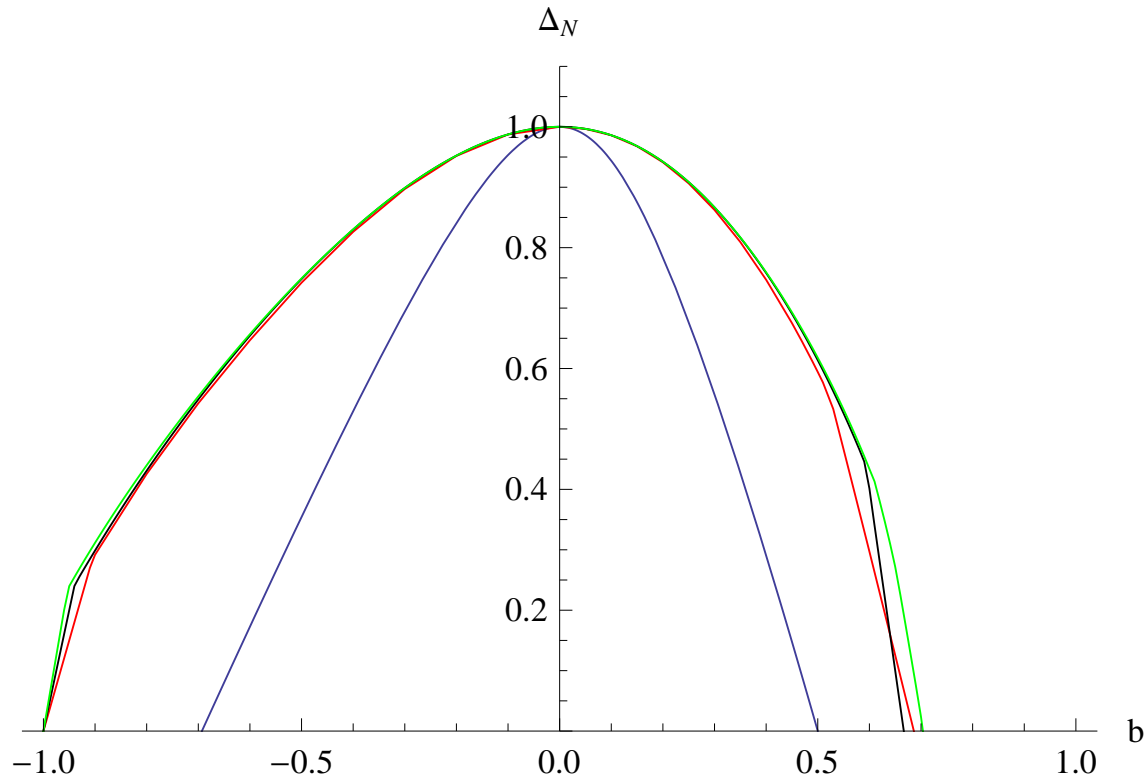
*3.3.2. Spin tubes* Several specific choices of the inter-trimer interaction matrix between the trimers correspond to so-called three-leg or triangular spin tubes. Such spin tubes have been widely considered in the literature, see e. g. [15].

*Spin tube I:* The choice of the inter-trimer interaction matrix

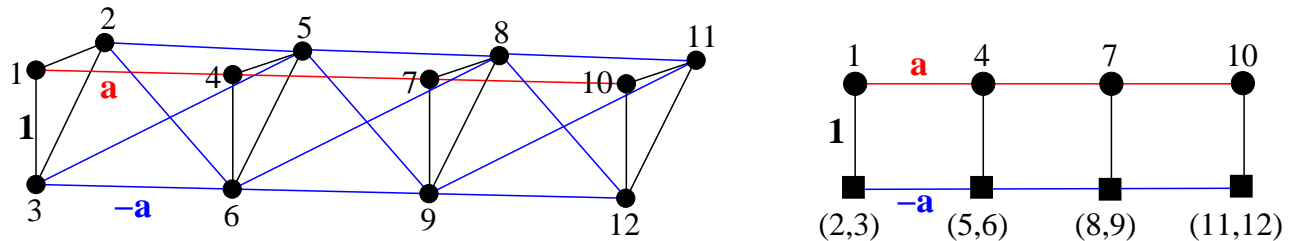
$$(J_{\delta,\epsilon}) = \frac{1}{2} \begin{pmatrix} a & 0 & 0 \\ 0 & -a & -a \\ 0 & -a & -a \end{pmatrix} \quad (25)$$

leads to a spin tube as shown figure 8. For the special kind of systems (25) it turns out that the chains have an additional symmetry, namely that certain composite spin squares (in figure 8 these are  $\tilde{S}_{23}^2, \tilde{S}_{56}^2$ , etc. ) commute with the Hamiltonian. Hence one can consider a simpler ladder model composed of spins and composite spins, see figure 8. This ladder is frustrated, since the upper and the lower leg exchange bonds have different sign. In the singlet product state  $\Phi$  the composite spins on the lower leg have the same spin quantum number  $s$  as the individual spins. Hence we have an effective spin- $s$  ladder, where the antiferromagnetically coupled rungs are in a local singlet state. Note that a similar exact singlet product state was also found for a spin-half ladder with one ferromagnetic leg and one antiferromagnetic leg [21].

We have numerically determined the critical values  $a_{\min}$  and  $a_{\max}$  where  $\Phi$  ceases to be the unique ground state with energy  $E_0 = -\frac{3N}{2}s(s+1)$ . These critical values depend on the number of spins  $3N$  and the spin quantum number  $s$ . The results are contained



**Figure 7.** The numerically calculated energy gap  $\Delta_N(b)$  of the chain of  $N$  corner sharing tetrahedra as a function of the coupling constant  $b$  for  $N = 2, 3, 4, 5$  and  $s = 1$ . The lower-most blue curve corresponds to  $N = 2$ ; the next curves correspond to  $N = 3$  (red),  $N = 4$  (black) and  $N = 5$  (green). According to corollary 2 of section 4.4 we have the rigorous bound  $\Delta_N \geq \Delta_2$  for all  $N = 3, 4, \dots$ , which is confirmed by these examples. The curves  $\Delta_N(b)$  show only small variations for  $N = 3, 4, 5$ . They seem to grow monotonically with  $N$  except for  $b > 0.64$  where the  $N = 3$  and the  $N = 4$  curves intersect. The parabolic form of the gap functions in the neighborhood of  $b = 0$  can be understood by virtue of 1st and 2nd order perturbation theory and considering local  $S = 1$  excitations for  $b = 0$  satisfying  $\Delta_N(0) = 1$ . The 1st order corrections vanish due to the balanced form of the inter-trimer Hamiltonian; the 2nd order contributions have a negative sign since the local excitations can be treated like ground states in the Hilbert space  $\Phi^\perp$ . Note that the perturbed local excitations need not be the competing ground states; this explains the kinks in the gap functions.



**Figure 8.** Example of a spin tube I (left) and an equivalent effective ladder of composite spins (right).

**Table 2.** Critical values of the coupling constant  $a$  corresponding to the chains of figure 8.

$3N$	$s$	$a_{\min}$	$a_{\max}$
12	1	-0.319	0.418
18	1	-0.330	0.419
12	2	-0.210	0.270

in table 2. In accordance with our general conjectures we find that the critical interval  $[a_{\min}, a_{\max}]$  shrinks when passing from  $s = 1$  to  $s = 2$  and slightly expands from  $N = 12$  to  $N = 18$ .

Based on the numerical data we have analyzed the competing states which become ground states for  $a < a_{\min}$  and  $a > a_{\max}$ . In the competing state for both cases the composite spins have the spin quantum number  $s + 1$ . As a result, the lower leg of the effective model carrying larger spins determines the magnetic ordering of the systems. While for positive  $a$  within both legs the spin-spin correlations are ferromagnetic in the competing state, one has a competing state with antiferromagnetic spin-spin correlations within both legs for negative  $a$ . Due to the antiferromagnetic rung coupling the total spin of the system is  $S = 0$  for  $a < a_{\min}$ , whereas the competing state is ferrimagnetic with  $S = N$  for  $a > a_{\max}$ .

*Spin tubes II:* The choice of the inter-trimer interaction matrix

$$(J_{\delta,\epsilon}) = \frac{1}{2} \begin{pmatrix} 0 & d & 0 \\ 0 & d & 0 \\ b & b+d & b \end{pmatrix} \quad (26)$$

leads to another spin tube, see figure 9. For this special kind of coupling it turns out that the chains have no additional symmetry (i.e. no composite spins are conserved), if both parameters  $b$  and  $d$  are non-zero. Nevertheless,  $\Phi$  will be the unique ground state for a convex neighborhood of the point  $b = d = 0$ . Our numerical results are contained in figure 10.

First, we notice that in the limits  $b = 0$  or  $d = 0$  some of the bonds are missing, and the model can be transformed to the chain of corner-sharing tetrahedra. As a trivial result the competing states and the corresponding transition points are the same as discussed in section 3.3.1. Consequently, the competing state at (and also in the vicinity of)  $b = 0$ ,  $d = -1$  and also  $d = 0$ ,  $b = -1$  is ferrimagnetic. In all the other areas we find numerically that the competing state is a non-trivial singlet state. However, its spin-spin correlations depend strongly on the position on the transition line shown in figure 10.



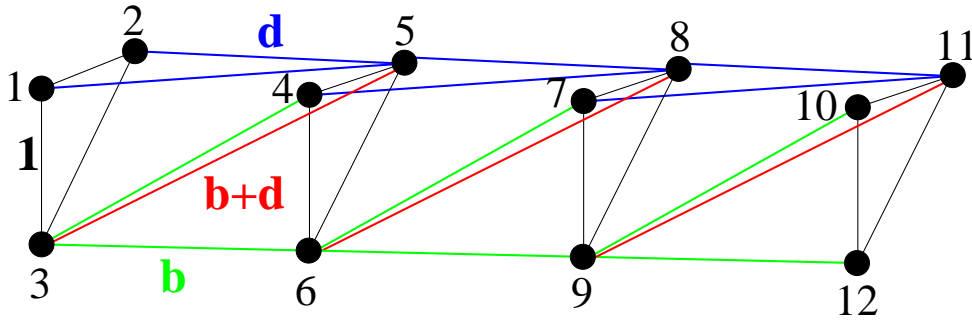
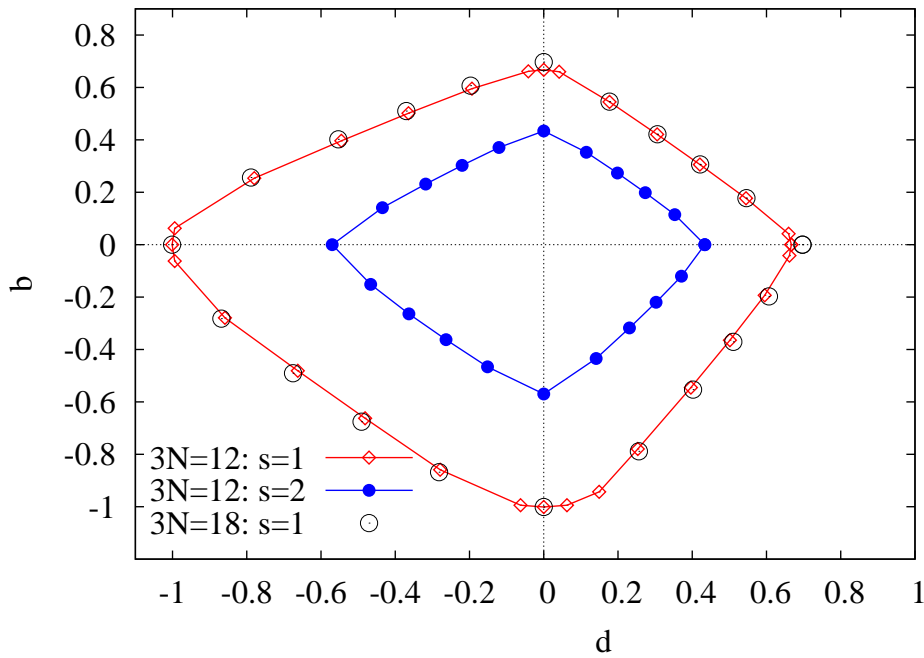


Figure 9. Example of a spin tube II.

Figure 10. Representation of the set of points  $\mathcal{T}^s$  with coordinates  $(b, d)$  such that  $\Phi$  will be a ground state of Hamiltonian corresponding to spin tube II shown in figure 9.

As for the previous examples, it is obvious from figure 10 that there is only a very weak dependence on the size of the system. Moreover, we observe an inclusion  $\mathcal{T}^2 \subset \mathcal{T}^1$ , which is compatible with the conjecture that the domain in the coordinate space  $(b, d)$  where  $\Phi$  will be a ground state shrinks with increasing spin quantum number  $s$ .

## 4. Rigorous results

### 4.1. Definitions

We recall the general definitions given in section 2. Analogous definitions hold for the classical case: Here the spin observables  $\mathbf{s}_\mu^d$  are unit vectors,  $H(\mathbb{J})^d$  is the Hamiltonian

function, defined on the  $3N$ -fold Cartesian product of unit spheres

$$\mathcal{P} \equiv \bigtimes_{\mu=1}^{3N} \mathcal{S}_{(\mu)}^2, \quad (27)$$

and  $\Phi^{cl} \subset \mathcal{P}$  is the set of all spin configurations satisfying

$$\mathbf{s}_{i0} + \mathbf{s}_{i1} + \mathbf{s}_{i2} = \mathbf{0} \text{ for all } i = 1, \dots, N. \quad (28)$$

Note that  $\Phi^{cl}$  as well as  $\Phi^s$  are invariant under rotations.  $\mathbb{J}$  is said to have the classical TGS property iff the minimum of  $H(\mathbb{J})$  is assumed for all  $\mathbf{s} \in \Phi^{cl}$ . In this case we write  $\mathbb{J} \in \mathcal{C}_{\Phi}^{cl} = \mathcal{C}_{\Phi}^{\infty}$ .

#### 4.2. Necessary conditions for TGS systems

Whereas a complete characterization of  $\mathcal{C}_{\Phi}^s$  seems to be possible only for small  $N$  and  $s$  or for the classical case  $s = \infty$ , one can prove a number of partial results, either necessary or sufficient conditions for  $\mathbb{J} \in \mathcal{C}_{\Phi}^s$ .

We have already mentioned the following result which gives a necessary condition for  $\mathbb{J} \in \mathcal{C}_{\Phi}^s$ :

**Theorem 1**  $\Phi$  is an eigenstate of  $H(\mathbb{J})$  iff

$$J_{i0,j0} + J_{i1,j1} = J_{i0,j1} + J_{i1,j0} \quad (29)$$

$$J_{i0,j0} + J_{i1,j2} = J_{i0,j2} + J_{i1,j0} \quad (30)$$

$$J_{i0,j0} + J_{i2,j1} = J_{i0,j1} + J_{i2,j0} \quad (31)$$

$$J_{i0,j0} + J_{i2,j2} = J_{i0,j2} + J_{i2,j0} \quad (32)$$

for all  $i < j = 2, \dots, N$ . Moreover, let  $\mathcal{DS}_0$  denote the space of all real  $3 \times 3$ -matrices with vanishing row and column sums, and  $\check{J}_{ij}$  the  $3 \times 3$ -matrix with entries  $J_{i\epsilon,j\delta}$ ,  $\epsilon, \delta = 0, 1, 2$ . Then the above four equations (29) - (32) are equivalent to the statement that  $\check{J}_{ij}$  is orthogonal to the space  $\mathcal{DS}_0$  w. r. t. the inner product  $\langle A, B \rangle = \text{Tr}(A^\top B)$ .

**Proof:** The second part of the theorem follows, since the equations (29)-(32) say that  $\check{J}_{ij}$  is orthogonal to the four matrices

$$\begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & -1 \\ -1 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 1 & -1 & 0 \\ 0 & 0 & 0 \\ -1 & 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} \quad (33)$$

which span  $\mathcal{DS}_0$ .

To prove the first part of the theorem we rewrite the Hamiltonian (27) in the form

$$\begin{aligned} H(\mathbb{J}) &= \sum_{\mu \neq \nu} J_{\mu\nu} \mathbf{s}_{\mu} \cdot \mathbf{s}_{\nu} \\ &= \sum_{i \neq j} \sum_{\epsilon, \delta=0}^2 J_{i\epsilon,j\delta} \mathbf{s}_{i\epsilon} \cdot \mathbf{s}_{j\delta} \end{aligned} \quad (34)$$

$$+ 2 \sum_{i=1}^N \left( J_{i0,i1} \mathbf{s}_{i0} \cdot \mathbf{s}_{i1} + J_{i0,i2} \mathbf{s}_{i0} \cdot \mathbf{s}_{i2} + J_{i1,i2} \mathbf{s}_{i1} \cdot \mathbf{s}_{i2} \right) \quad (35)$$

$$\equiv \sum_{i < j} \overline{H}_{ij}, \quad (36)$$

where the distribution of the terms of the second sum in (35) to the terms  $\overline{H}_{ij}$  is arbitrary. We have  $\overline{H}_{ij} = \widetilde{H}_{ij} \otimes \mathbb{1}^{(ij)}$  such that  $\widetilde{H}_{ij}$  acts on  $\mathcal{H}_{ij} = \mathcal{H}_i \otimes \mathcal{H}_j$  and  $\mathbb{1}^{(ij)}$  on the remaining factors. Recall that the trimerized state has the form

$$\Phi = \bigotimes_{i=1}^N [i0, i1, i2], \quad (37)$$

where  $[i0, i1, i2]$  denotes the AF trimer ground state in  $\mathcal{H}_i = \mathcal{H}_{i0} \otimes \mathcal{H}_{i1} \otimes \mathcal{H}_{i2}$ . The following lemma can be proven completely analogous to lemma 2 in [9]

**Lemma 1**  $\Phi$  is an eigenstate of  $\widetilde{H}(\mathbb{J})$  iff  $[i0, i1, i2] \otimes [j0, j1, j2]$  is an eigenstate of  $\widetilde{H}_{ij}$  for all  $i < j = 2, \dots, N$ .

In view of this lemma we only need to consider the case of  $N = 2$  trimers with indices  $i < j$  in the remaining part of the proof. We set  $\phi = [i0, i1, i2]$  and rewrite the indices according to

$$(i0) \equiv 1, (i1) \equiv 2, (i2) \equiv 3, \quad (j0) \equiv 4, (j1) \equiv 5, (j2) \equiv 6. \quad (38)$$

Since all summands in

$$0 = \langle \phi | S_{123}^2 | \phi \rangle = \sum_{i=1}^3 \langle \phi | (\mathbf{s}_1^{(i)} + \mathbf{s}_2^{(i)} + \mathbf{s}_3^{(i)})^2 | \phi \rangle \quad (39)$$

are non-negative, we conclude  $\|(\mathbf{s}_1^{(i)} + \mathbf{s}_2^{(i)} + \mathbf{s}_3^{(i)}) \phi\|^2 = 0$ , i. e.  $(\mathbf{s}_1^{(i)} + \mathbf{s}_2^{(i)} + \mathbf{s}_3^{(i)}) \phi = 0$  for  $i = 1, 2, 3$ . Further,  $(\mathbf{s}_1 + \mathbf{s}_2 + \mathbf{s}_3) \cdot \mathbf{s}_\nu (\phi \otimes \phi) = 0$  for  $\nu = 4, 5, 6$ . Hence, for arbitrary  $\Psi \in \mathcal{H}_{ij}$ , the matrix  $D$  with entries

$$D_{\mu\nu} = \langle \Psi | \mathbf{s}_\mu \cdot \mathbf{s}_{\nu+3} (\phi \otimes \phi) \rangle \quad \mu, \nu = 1, 2, 3, \quad (40)$$

has vanishing row and column sums, i. e.  $D \in \mathcal{DS}_0$ .  $\phi \otimes \phi$  is an eigenstate of  $\widetilde{H}(\mathbb{J})$  iff  $\widetilde{H}(\phi \otimes \phi) = 0$  with  $\widetilde{H} = \sum_{\mu, \nu=1}^3 \check{J}_{\mu\nu} \mathbf{s}_\mu \cdot \mathbf{s}_{\nu+3}$ . This in turn is equivalent to  $\langle \Psi | \widetilde{H}(\phi \otimes \phi) \rangle = 0$  for all  $\Psi \in \mathcal{H}_{ij}$ , or  $\langle \check{J}, D \rangle = \sum_{\mu, \nu=1}^3 \check{J}_{\mu\nu} D_{\mu\nu} = 0$ , i. e.  $\check{J}$  is orthogonal to all matrices in  $\mathcal{DS}_0$  which can be written in the form (40).

It remains to show that there exist enough  $\Psi \in \mathcal{H}_{ij}$  such that the matrices of the form (40) constitute a basis of  $\mathcal{DS}_0$ . Note that for all  $s = 1, 2, 3, \dots$   $\phi$  has a non-vanishing scalar product with the basis vector  $e = |1, -1, 0\rangle$ . Choose  $\Psi = e \otimes e$  and consider the corresponding matrix (40)  $D^{(1)}$  with entries  $D_{\mu\nu}^{(1)} = \langle \Psi | \mathbf{s}_\mu \cdot \mathbf{s}_{\nu+3} (\phi \otimes \phi) \rangle = \langle e | \mathbf{s}_\mu \phi \rangle \langle e | \mathbf{s}_\nu \phi \rangle$ . First, we conclude that  $\langle e | \mathbf{s}_\mu^{(1)} \phi \rangle = \langle e | \mathbf{s}_\mu^{(2)} \phi \rangle = 0$  since  $\mathbf{s}_\mu^{(1)}$  and  $\mathbf{s}_\mu^{(2)}$  change the spin quantum number  $S_{123}^{(3)}$  which is 0 for  $e$  and  $\phi$ . Second,  $\mathbf{s}_3^{(3)} e = 0$ ,

$$\text{hence } D^{(1)} = d_1 \begin{pmatrix} 1 & -1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad d_1 \neq 0. \quad \text{The remaining matrices of the basis in (33)}$$

are similarly obtained by choosing  $\Psi = |1, -1, 0, 1, 0, -1\rangle$ ,  $\Psi = |1, 0, -1, 1, -1, 0\rangle$ , and  $\Psi = |1, 0, -1, 1, 0, -1\rangle$ . This concludes the proof of theorem 1.  $\blacksquare$

Since (29)-(32) is a system of four linearly independent equations, the set of all real, symmetric  $3N \times 3N$ -matrices satisfying (29)-(32) and  $J_{\mu\mu} = 0$  for all  $\mu = 1, \dots, 3N$  will be a linear space of dimension  $3N + 5\binom{N}{2} = \frac{N}{2}(5N+1)$ , denoted by  $\mathcal{J}_\Phi$ . The set  $\mathcal{C}_\Phi$  of TGS systems will form a closed convex cone embedded in the linear space  $\mathcal{J}_\Phi$ , see [9]. If  $\Phi$  is an eigenstate of  $\tilde{H}(\mathbb{J})$  it is straightforward to calculate the corresponding eigenvalues, since  $\langle \Phi | \tilde{\mathbf{s}}_{i\delta} \cdot \tilde{\mathbf{s}}_{j\epsilon} | \Phi \rangle = 0$  for  $i \neq j$ :

**Corollary 1** *If  $\Phi$  is an eigenstate of  $\tilde{H}(\mathbb{J})$  then*

$$\tilde{H}(\mathbb{J})\Phi = -s(s+1) \left( \sum_{i=1}^N J_{i0,i1} + J_{i0,i2} + J_{i1,i2} \right) \Phi. \quad (41)$$

In the classical case we have similar but stronger results: The conditions (29)-(32) can be strengthened to a uniform coupling condition:

**Theorem 2** *If  $\mathbb{J} \in \mathcal{C}_\Phi^{cl}$  then the coupling constants do not depend on  $\delta, \epsilon$ , i. e.*

$$J_{i\delta,i\epsilon} \equiv J_i > 0 \quad (42)$$

and

$$J_{i\delta,j\epsilon} \equiv \varepsilon_{ij} \quad (43)$$

for all  $\delta, \epsilon = 0, 1, 2$  and  $i < j = 2, \dots, N$ .

Consequently, we will denote by  $\mathcal{J}_\Phi^\infty \equiv \mathcal{J}_\Phi^{cl}$  the linear space of all real, symmetric,  $3N \times 3N$ -matrices  $\mathbb{J}$  with vanishing diagonals and satisfying (42) (except  $J_i > 0$ ) and (43).

**Proof** of theorem 2: The ground states of classical Heisenberg systems satisfy

$$\sum_{\nu} J_{\mu\nu} \mathbf{s}_\nu = \kappa_\mu \mathbf{s}_\mu, \quad \mu = 1, \dots, 3N, \quad (44)$$

see eq. (16) in [22]. This equation results from the condition that the energy  $H = \sum_{\mu\nu} J_{\mu\nu} \mathbf{s}_\mu \cdot \mathbf{s}_\nu$  assumes a minimum, subject to the constraints  $\mathbf{s}_\mu \cdot \mathbf{s}_\mu = 1$ . Here the  $\kappa_\mu$ ,  $\mu = 1, \dots, 3N$  appear as the Lagrange parameters corresponding to these constraints. We choose  $\mu = (i, 0)$  and rewrite (44) in the form

$$\sum_{j(\neq i), \epsilon} J_{i0,j\epsilon} \mathbf{s}_{j\epsilon} + J_{i0,i1} \mathbf{s}_{i1} + J_{i0,i2} \mathbf{s}_{i2} = \kappa_{i0} \mathbf{s}_{i0}. \quad (45)$$

It is clear, by definition of classical TGS systems, that the contributions from different trimers with index  $j \neq i$  in (45) can be rotated independently. These rotated contributions cannot be compensated by variations of  $\kappa_{i0}$  unless  $\sum_{\epsilon} J_{i0,j\epsilon} \mathbf{s}_{j\epsilon}$  vanishes for all  $j \neq i$ . Choosing  $s_{j0}^{(1)} = -s_{j1}^{(1)} = \frac{1}{2}$  and  $s_{j2}^{(1)} = 0$  yields  $J_{i0,j1} = J_{i0,j2}$ . Similar arguments apply to the other equations which say that the coupling between different trimers must be uniform.

To prove uniform coupling within the trimers we reconsider (45) in the form  $J_{i0,i1} \mathbf{s}_{i1} +$

$J_{i0,i2}\mathbf{s}_{i2} = \kappa_{i0}\mathbf{s}_{i0}$ . The special choice  $s_{i1}^{(1)} = -s_{i2}^{(1)} = \frac{1}{2}$  and  $s_{i0}^{(1)} = 0$  again yields  $J_{i0,i1} = J_{i0,i2}$  and analogously for the other equations.

The previous considerations show that for classical trimerized ground states the Hamiltonian assumes the value  $E = -3 \sum_{i=1}^N J_i$ . If one of the  $J_i$  would be negative, say  $J_1 < 0$ , one could lower the energy by choosing  $\mathbf{s}_{10} = \mathbf{s}_{11} = \mathbf{s}_{12}$ . Hence all  $J_i \geq 0$  and the proof is complete.  $\blacksquare$

### 4.3. Systems close to unconnected trimers

Let  $\overset{\circ}{\mathbb{J}}$  denote the matrix of an *unconnected TGS system*, i. e.

$(\overset{\circ}{J}_{i0,i1}, \overset{\circ}{J}_{i0,i2}, \overset{\circ}{J}_{i1,i2}) \in \mathcal{C}_{\Phi_i}^s$  for all  $i = 1, \dots, N$  where  $\Phi_i$  denote the local trimerized ground states. All other matrix elements  $\overset{\circ}{J}_{i\delta,j\epsilon}$  with  $i \neq j$  vanish. Of course,  $\overset{\circ}{\mathbb{J}} \in \mathcal{C}_{\Phi}^s$  and hence the next lowest energy eigenvalue  $E_1$  satisfies

$$E_1 = E_0 + \varepsilon \equiv \langle \Phi | H(\overset{\circ}{\mathbb{J}}) | \Phi \rangle + \varepsilon, \quad \varepsilon > 0. \quad (46)$$

By continuity arguments, a small neighborhood of  $\overset{\circ}{\mathbb{J}}$  still consists of TGS systems. We want to derive a more quantitative result and consider an inter-trimer  $3N \times 3N$  symmetric coupling matrix  $\Delta \neq 0$  which has to be “small” in a certain sense. As a measure of “smallness” of  $\Delta$  we will use  $|\delta_{\min}|$  where  $\delta_{\min}$  denotes the lowest eigenvalue of the matrix  $\Delta$ . Note that  $\text{Tr } \Delta = 0$ , hence  $\delta_{\min} < 0$  and the highest eigenvalue  $\delta_{\max}$  of  $\Delta$  satisfies  $0 < \delta_{\max} \leq (3N - 1)|\delta_{\min}|$ . It is clear that the size of the neighborhood of  $\overset{\circ}{\mathbb{J}}$  depends on the energy gap of  $H(\overset{\circ}{\mathbb{J}})$  which explains the  $\varepsilon$  in the numerator of (47):

**Proposition 1** *Let  $\overset{\circ}{\mathbb{J}}$  be an unconnected TGS system and  $\mathbb{J} = \overset{\circ}{\mathbb{J}} + \Delta$ ,  $\Delta \in \mathcal{J}_{\Phi}$  such that*

$$|\delta_{\min}| \leq \frac{\varepsilon}{3Ns(s+1)}, \quad (47)$$

*where  $\delta_{\min}$  denotes the lowest eigenvalue of  $\Delta$ . Then  $\mathbb{J} \in \mathcal{C}_{\Phi}^s$ .*

Although the proof of proposition 1 is largely analogous to that of proposition 3 in [9], we will give it here for sake of convenience. The  $s$ -dependence of the bound in (47) supports the conjecture that the cones  $\mathcal{C}_{\Phi}^s$  shrink with increasing  $s$ .

**Proof** of proposition 1: Let  $\Psi$  be any normalized state satisfying  $\Psi \perp \Phi$ . It follows that

$$\langle \Psi | H(\overset{\circ}{\mathbb{J}}) | \Psi \rangle \geq E_1. \quad (48)$$

Further,

$$\langle \Psi | H(\Delta) | \Psi \rangle = \sum_{\mu, \nu} \Delta_{\mu, \nu} \langle \Psi | \mathfrak{s}_{\mu} \cdot \mathfrak{s}_{\nu} | \Psi \rangle \equiv \text{Tr } \Delta S \quad (49)$$

$$\geq \delta_{\min} \text{Tr } S = \delta_{\min} \sum_{\mu=1}^{3N} \langle \Psi | \mathfrak{s}_{\mu}^2 | \Psi \rangle = 3N\delta_{\min}s(s+1) \quad (50)$$

$$\geq -\varepsilon, \quad (51)$$

where the last inequality follows from (47) and  $\delta_{\min} < 0$ . It follows that

$$\langle \Psi | H(\mathbb{J}) | \Psi \rangle = \langle \Psi | H(\overset{\circ}{\mathbb{J}}) | \Psi \rangle + \langle \Psi | H(\Delta) | \Psi \rangle \quad (52)$$

$$\geq E_1 - \varepsilon = E_0, \quad (53)$$

hence  $\Phi$  will be a ground state of  $H(\mathbb{J})$ . This concludes the proof of proposition 1.  $\blacksquare$

An important special case of proposition 1 is the case of an *unconnected homogeneous TGS system*, i. e.  $\overset{\circ}{J}_{i0,i1} = \overset{\circ}{J}_{i0,i2} = \overset{\circ}{J}_{i1,i2} \equiv \lambda_i > 0$  for all  $i = 1, \dots, N$ . In this case

$$\varepsilon = 2\lambda \equiv 2 \min\{\lambda_i | i = 1, \dots, N\}. \quad (54)$$

One of the simplest potential TGS systems  $\mathbb{J}(\epsilon)$ , see figure 11, shows an interesting effect: For given  $s$  and sufficiently small  $\epsilon$  it is a TGS system by virtue of proposition 1. But if  $\epsilon > 0$  is fixed and  $s$  increases, it eventually loses the TGS property. Otherwise we would get a contradiction since  $\mathbb{J}(\epsilon) \notin \mathcal{C}_{\Phi}^{\text{cl}}$  by theorem 2 and the (normalized) ground state energy must converge for  $s \rightarrow \infty$  towards its classical value as a consequence of the Berezin/Lieb inequality [23]

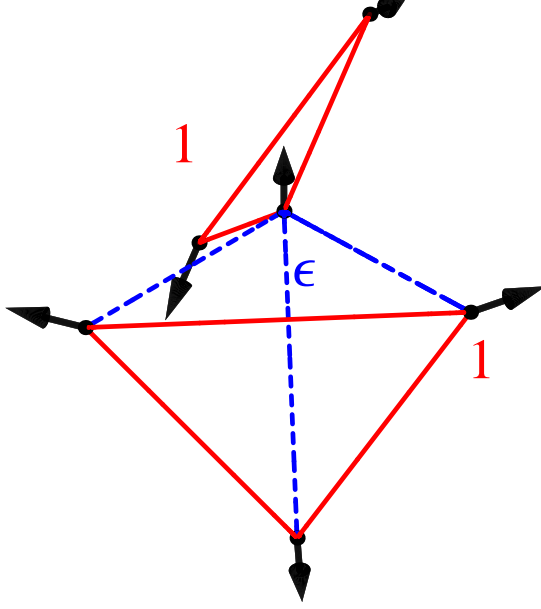
$$(s+1)^2 E_{\min}^{\text{cl}} \leq E_{\min} \leq s^2 E_{\min}^{\text{cl}}. \quad (55)$$

#### 4.4. The TGS chain

A TGS chain consists of  $N$  copies of trimers such that the intra-trimer and inter-trimer coupling is invariant under one-dimensional translations and  $\Phi$  is a ground state with energy  $\tilde{E}_0(N)$ . A first question is whether for a given coupling the system remains a TGS chain for all  $N \in \mathbb{N}, N \geq 2$ . If this is the case, one may ask if the difference  $\Delta_N$  between the next-lowest eigenvalue  $\tilde{E}_1(N)$  and  $\tilde{E}_0(N)$  has a positive lower bound independent of  $N$ . In this case one says that  $\Phi$  is a *gapped* ground state. Here we ignore further questions concerning the limit of  $\Delta_N$  for  $N \rightarrow \infty$  and confine ourselves to the existence of a gap for TGS chains.

We will prove our result in a slightly more general context. Correspondingly, some of the general definitions of the paper are abolished in the following theorem. We consider a Hamiltonian  $H = \sum_{i=1}^N H_i$  where the  $H_i$  live in Hilbert spaces  $\mathcal{H}_i \otimes \mathcal{H}_{i+1}$  and the total Hamiltonian  $H$  in  $\mathcal{H} = \bigotimes_{i=1}^N \mathcal{H}_i$ . All Hilbert spaces  $\mathcal{H}_i$  are copies of one finite-dimensional Hilbert space. These and the following definitions are to be understood in the sense of cyclic boundary conditions  $N+1 \equiv N$ . Moreover, if  $T$  is the unitary translation operator in  $\mathcal{H}$  shifting the tensor factors cyclically and hence satisfying  $T^N = \mathbb{1}$ , we will assume  $T H_i T^* = H_{i+1}$  and hence  $[T, H] = 0$ .

**Theorem 3** *Let  $\Phi_i \in \mathcal{H}_i$  be normalized and  $\Phi_i \otimes \Phi_{i+1}$  be the unique ground state of  $H_i$  with eigenvalue  $E_0$  and the next-lowest eigenvalue being  $E_1 = E_0 + \delta$ ,  $\delta > 0$ . Then  $\Phi = \bigotimes_{i=1}^N \Phi_i$  will be the unique ground state of  $H$  with eigenvalue  $\tilde{E}_0 = N E_0$  and the next-lowest eigenvalue satisfies  $\tilde{E}_1 \geq \tilde{E}_0 + 2\delta$ .*



**Figure 11.** This system cannot be a TGS system for fixed  $\epsilon > 0$  and arbitrary  $s$ , since its classical limit is not TGS. The classical ground state corresponding to an energy  $E_0 = -3 - \frac{\epsilon^2}{9}$  is indicated by small arrows.

**Proof:** The first claim follows immediately by

$$\begin{aligned}
 H\Phi &= \sum_{i=1}^N H_i \Phi = \sum_{i=1}^N \Phi_1 \otimes \cdots \otimes H_i(\Phi_i \otimes \Phi_{i+1}) \otimes \cdots \otimes \Phi_N \\
 &= \sum_{i=1}^N E_0 \Phi = N E_0 \Phi = \tilde{E}_0 \Phi
 \end{aligned} \tag{56}$$

and  $N E_0$  being an obvious lower bound of  $H$ .

Let  $\Psi \in \mathcal{H}$  be the eigenvector of  $H$  belonging to the next-lowest eigenvalues  $\tilde{E}_1 \geq \tilde{E}_0$ . We may assume that

$$\Psi \perp \Phi \text{ and } T\Psi = e^{i\alpha}\Psi, \quad \alpha = 2\pi k/N, \quad k \in \mathbb{Z}. \tag{57}$$

Our aim is to show  $\tilde{E}_1 \geq \tilde{E}_0 + 2\delta$ . Let  $|\mu\rangle, \mu = 0, 1, 2, \dots$  denote the eigenbasis of  $H_i$  in  $\mathcal{H}_i \otimes \mathcal{H}_{i+1}$  such that  $|0\rangle = \Phi_i \otimes \Phi_{i+1}$ .  $|\mu, K\rangle$  denotes a corresponding product basis in  $\mathcal{H}$ , where  $K$  stands for some multi-index of quantum numbers. Moreover, we consider the reduced density operator  $W_\Psi^i$  in  $\mathcal{H}_i \otimes \mathcal{H}_{i+1}$  defined by the partial trace

$$\langle \mu | W_\Psi^i | \nu \rangle = \sum_K \langle \mu, K | \Psi \rangle \langle \Psi | \nu, K \rangle. \tag{58}$$

Then we conclude

$$\tilde{E}_1 = \langle \Psi | H | \Psi \rangle = \sum_{i=1}^N \langle \Psi | H_i | \Psi \rangle \quad (59)$$

$$= \sum_{i=1}^N \text{Tr} (H_i W_\Psi^i) \quad (60)$$

$$= \sum_{i,\mu} \text{Tr} (E_\mu |\mu\rangle \langle \mu| W_\Psi^i) \quad (61)$$

$$= \sum_{i,\mu} E_\mu \langle \mu | W_\Psi^i | \mu \rangle \quad (62)$$

$$= \sum_i \left( E_0 \langle 0 | W_\Psi^i | 0 \rangle + \sum_{\mu=1,2,\dots} E_\mu \langle \mu | W_\Psi^i | \mu \rangle \right) \quad (63)$$

$$\geq \sum_i \left( E_0 \langle 0 | W_\Psi^i | 0 \rangle + (E_0 + \delta) \sum_{\mu=1,2,\dots} \langle \mu | W_\Psi^i | \mu \rangle \right). \quad (64)$$

**Lemma 2**  $\langle 0 | W_\Psi^i | 0 \rangle \leq 1 - \frac{2}{N}.$  (65)

For the proof of the lemma we use an arbitrary orthonormal basis  $|n\rangle$ ,  $n = 0, 1, 2, \dots$  in  $\mathcal{H}_i$  such that  $|0\rangle = \Phi_i$  and  $T$  operates as a cyclic shift operator in the corresponding product basis in  $\mathcal{H}$ . Hence  $\langle 0 | W_\Psi^i | 0 \rangle$  will be rewritten as  $\langle 0, 0 | W_\Psi^i | 0, 0 \rangle$ . In this notation we have  $\Phi = |0, 0, \dots, 0\rangle$ . Due to translational symmetry the term (65) does not depend on  $i$ , hence we may take  $i = 1$  in what follows. We conclude

$$\langle 0, 0 | W_\Psi^i | 0, 0 \rangle = \sum_K |\langle \Psi | 0, 0, K \rangle|^2 \quad (66)$$

and

$$\begin{aligned} 1 = \text{Tr} W_\Psi^i &= \sum_{n_3, n_4, \dots} |\langle \Psi | 0, 0, n_3, n_4, \dots \rangle|^2 + \sum_{n_1, n_2, \dots} |\langle \Psi | n_1, n_2, \dots \rangle|^2 \\ &\equiv s_0 + s_1. \end{aligned} \quad (67)$$

The first sum  $s_0$  in (67) runs through all sequences  $0, 0, n_3, n_4, \dots$  excluding the value  $n_3 = n_4 = \dots = 0$ , since  $\langle \Psi | \Phi \rangle = 0$ . Equivalently, we will say that it runs through all states  $\psi = |0, 0, n_3, n_4, \dots\rangle \in \mathcal{B}_0$ . The second sum  $s_1$  in (67) runs through all sequences  $n_1, n_2, \dots$  except those with  $n_1 = n_2 = 0$ , or, equivalently, through all states  $\psi = |n_1, n_2, \dots\rangle \in \mathcal{B}_1$ . Thus the total sum in (67) runs through an orthonormal basis  $\mathcal{B} = \mathcal{B}_0 \cup \mathcal{B}_1$  of  $\mathcal{H}' \equiv \{\psi \in \mathcal{H} | \langle \psi | \Phi \rangle = 0\}$ .

We consider on  $\mathcal{B}$  the equivalence relation  $\psi_1 \sim \psi_2 \Leftrightarrow \psi_1 = T^a \psi_2$ ,  $a \in \mathbb{Z}$ , and denote by  $\Lambda = \mathcal{B}/\sim$  the corresponding set of equivalence classes or “orbits”. Due to (57) all states  $\psi$  in the same orbit  $\lambda$  yield the same value

$$t_\lambda \equiv |\langle \Psi | \psi \rangle|^2 = |\langle \Psi | T^a \psi \rangle|^2, \quad a \in \mathbb{Z}. \quad (68)$$

For each orbit  $\lambda \in \Lambda$  let  $N_\lambda \equiv |\lambda|$  denote its length. For most orbits we have  $N_\lambda = N$ , but in general  $N_\lambda$  will be a divisor of  $N$ . For example, if  $N = 6$  and  $|1, 2, 3, 1, 2, 3\rangle \in \lambda$



then  $N_\lambda = 3$ . We define  $N_\lambda^{(k)} \equiv |\lambda \cap \mathcal{B}_k|$ ,  $k = 0, 1$ , and obtain the following equations:

$$N_\lambda = N_\lambda^{(0)} + N_\lambda^{(1)}, \quad (69)$$

$$s_0 = \sum_{\lambda \in \Lambda} t_\lambda N_\lambda^{(0)}, \quad (70)$$

$$s_1 = \sum_{\lambda \in \Lambda} t_\lambda N_\lambda^{(1)}. \quad (71)$$

If  $N_\lambda = N$  any basis vector  $\psi = |n_1, n_2, n_3, n_4, \dots\rangle \in \lambda$  has exactly  $N$  mutually orthogonal translations. Note that at least one  $n_j$ ,  $1 \leq j \leq N$  must be non-zero since  $\psi \neq \Phi = |0, 0, \dots, 0\rangle$ . Hence at least two translations of  $\psi$  belong to  $\mathcal{B}_1$ , namely those where  $j$  is shifted to 1 or 2. It follows that  $N_\lambda^{(1)} \geq 2$  and hence  $N_\lambda^{(0)} \leq N - 2$ . Similarly, in the general case of  $1 < N_\lambda \leq N$  we also have  $N_\lambda^{(1)} \geq 2$  and hence  $N_\lambda^{(0)} \leq N_\lambda - 2 \leq N - 2$ . In the case  $N_\lambda = 1$ , that is,  $\psi = |n, n, \dots, n\rangle$ ,  $n > 0$  we have  $N_\lambda^{(1)} = 1$  and  $N_\lambda^{(0)} = 0$ . This case has to be treated separately. We write  $\lambda \in \Lambda_1$  iff  $N_\lambda = 1$  and  $\lambda \in \Lambda_>$  iff  $N_\lambda > 1$  and conclude

$$s_0 = \sum_{\lambda \in \Lambda_>} t_\lambda N_\lambda^{(0)} \leq (N - 2) \sum_{\lambda \in \Lambda_>} t_\lambda, \quad (72)$$

$$s_1 = \sum_{\lambda \in \Lambda_1} t_\lambda + \sum_{\lambda \in \Lambda_>} t_\lambda N_\lambda^{(1)} \geq 2 \sum_{\lambda \in \Lambda_>} t_\lambda, \quad (73)$$

which for  $\sum_{\lambda \in \Lambda_>} t_\lambda > 0$  implies

$$\frac{s_1}{s_0} \geq \frac{2}{N - 2}. \quad (74)$$

If  $\sum_{\lambda \in \Lambda_>} t_\lambda = 0$  then  $s_0 = 0$  and (65) follows immediately. From (74) we infer

$$\frac{1}{s_0} = \frac{s_0 + s_1}{s_0} = 1 + \frac{s_1}{s_0} \geq 1 + \frac{2}{N - 2} = \frac{N}{N - 2} \quad (75)$$

and

$$s_0 \leq \frac{N - 2}{N} = 1 - \frac{2}{N}, \quad (76)$$

$$s_1 \geq \frac{2}{N}, \quad (77)$$

which concludes the proof of the lemma. ■

To complete the proof of theorem 3 we consider

$$1 = \text{Tr } W_\Psi^i = \langle 0 | W_\Psi^i | 0 \rangle + \sum_{\mu=1,2,\dots} \langle \mu | W_\Psi^i | \mu \rangle = s_0 + s_1 \quad (78)$$

and rewrite (64) as

$$\tilde{E}_1 \geq \sum_{i=1}^N (E_0 s_0 + (E_0 + \delta) s_1) = \sum_{i=1}^N (E_0 + \delta s_1) \quad (79)$$

$$= N E_0 + N \delta s_1 \geq N E_0 + N \delta \frac{2}{N} = \tilde{E}_0 + 2 \delta, \quad (80)$$

where we have used (77) which is equivalent to (65). ■

The generalization of theorem 3 ( $d = 1$ ) to square ( $d = 2$ ) and cubic ( $d = 3$ ) lattices is obvious but will not be considered here. We only note that in this case the energy gap is bounded from below by  $2^d \delta$  for  $d = 1, 2, 3$ .

In order to apply theorem 3 to trimer chains we will take

$$H = H^{(N)} = \sum_{i=1}^N H_i \equiv \sum_{i=1}^N \sum_{\delta, \epsilon=0}^2 \left( \frac{1}{2} \overset{\circ}{J}_{\delta\epsilon} \left( \mathbf{s}_{i,\delta} \cdot \mathbf{s}_{i,\epsilon} + \mathbf{s}_{i+1,\delta} \cdot \mathbf{s}_{i+1,\epsilon} \right) + \check{J}_{\delta\epsilon} \mathbf{s}_{i,\delta} \cdot \mathbf{s}_{i+1,\epsilon} \right), \quad (81)$$

where the  $\check{J}_{\delta\epsilon}$  satisfy the conditions of theorem 1 and the Hilbert spaces  $\mathcal{H}_i$ ,  $i = 1, \dots, N$  are chosen appropriately. Of course,  $\Phi_i = [i_0, i_1, i_2]$ .

The  $3 \times 3$ -matrix  $\check{J}$  contains five independent real numbers and may thus be considered as a vector of  $\mathbb{R}^5$ . We will fix the values of the intra-trimer coupling  $\overset{\circ}{J}_{\delta\epsilon}$  such that the open convex set

$$\mathcal{T} \equiv \{ \check{J} | H_i \text{ has the unique ground state } [i_0, i_1, i_2] \} \subset \mathbb{R}^5 \quad (82)$$

is non-empty. Hence the energy gap of  $H_i$ ,  $E_1 - E_0 = \delta(\check{J})$  varies over  $\mathcal{T}$  but remains positive there. Then theorem 3 shows that  $H^{(N)}$  remains a TGS chain for all values  $\check{J} \in \mathcal{T}$  and all  $N \in \mathbb{N}$ . Moreover, the energy gap  $\Delta_N(\check{J}) = \tilde{E}_1(N) - \tilde{E}_0(N)$  satisfies  $\Delta_N(\check{J}) \geq 2\delta(\check{J})$ , hence  $\Phi$  is a gapped ground state in this case. Note that, due to the cyclic boundary conditions, we have  $H^{(2)} = 2H_1$ , hence  $\Delta_2(\check{J}) = 2\delta(\check{J})$ . We summarize:

**Corollary 2** *Let  $H^{(N)}$  be the Hamiltonian of a trimer chain according to (81) and the intra-trimer coupling  $\overset{\circ}{J}$  be chosen such that (82) is non-empty. Then  $H^{(N)}$  will be a TGS chain for all  $\check{J} \in \mathcal{T}$  and all  $N = 2, 3, \dots$  and its unique ground state  $\Phi$  possesses an energy gap satisfying  $\Delta_N(\check{J}) \geq \Delta_2(\check{J})$ .*

#### 4.5. The classical case

In the classical case it is possible to completely characterize all TGS systems. Recall that  $\epsilon_{ij} = \epsilon_{ji}$  denotes the uniform interaction strength between two trimers and  $J_i$  that within the trimers according to theorem 2. For any  $\mathbb{J} \in \mathcal{J}_\Phi^{cl}$  we define an  $N \times N$ -matrix  $\mathbb{G}(\mathbb{J})$  with entries

$$G_{ii} = J_i \text{ for all } i = 1, \dots, N, \quad (83)$$

$$G_{ij} = \epsilon_{ij} \text{ for all } i \neq j = 1, \dots, N. \quad (84)$$

Then we have the following result:

**Theorem 4** *Let  $\mathbb{J} \in \mathcal{J}_\Phi^{cl}$ , then  $\mathbb{J} \in \mathcal{C}_\Phi^{cl}$  iff  $\mathbb{G}(\mathbb{J})$  is positive semi-definite.*

Recall that  $\mathbb{G}(\mathbb{J}) \geq 0$  iff the  $N$  principal minors  $\det(G_{ij})_{i,j=1,\dots,n} \geq 0$  for  $n = 1, \dots, N$ . Hence for classical spin systems the TGS property can be checked by testing  $N$  inequalities.

This result is also relevant for quantum spin systems, since we have the following:

**Proposition 2**  $\mathcal{C}_\Phi^{cl} \subset \mathcal{C}_\Phi^s$  for all  $s = 1, 2, 3, \dots$

Again, the proofs of theorem 4 and proposition 2 are analogous to those given in sections 5.4 and 5.7 of [9].

### Appendix: Another eigenstate for the trimer pair

We reconsider the system of two trimers in section 3.2 with the special coupling

$$J_{12} = J_{13} = J_{23} = J_{45} = J_{46} = J_{56} = \frac{1}{2}, \quad (85)$$

$$J_{14} = -J_{26} = -J_{36} = -J_{25} = -J_{35} = \frac{a}{2}, \quad a < 0, \quad (86)$$

and the remaining coupling constants vanishing. We want to calculate a competing eigenstate  $\Psi$  which gives a lower energy than the trimerized state  $\Phi$  for  $a < a_{\text{crit}}$ .

As usual, we denote the composite spin of a subsystem by subscripts, e. g.  $\tilde{S}_{123}^2 = (\tilde{s}_1 + \tilde{s}_2 + \tilde{s}_3)^2$  with eigenvalues  $S_{123}(S_{123} + 1)$ . Recall that it is possible to construct orthonormal bases  $\mathcal{B}_T$  for the Hilbert space belonging to a spin system by means of “coupling schemes”  $T$ . For example, the coupling scheme  $1 \rightarrow 12 \rightarrow 123$  yields the common eigenbase of the composite spin squares  $\tilde{S}_{12}^2, \tilde{S}_{123}^2$  and the 3-component of the total spin  $\tilde{S}_{123}^{(3)}$ . It may happen that some state  $\Psi$  belongs to different  $\mathcal{B}_T$ ’s. In this case  $\Psi$  will be a common eigenvector of all composite spin squares corresponding to the different coupling schemes  $T$ . For example, the  $S = 0$  ground state  $[1, 2, 3]$  of a uniform AF trimer belongs to both coupling schemes  $1 \rightarrow 12 \rightarrow 123$  and  $1 \rightarrow 13 \rightarrow 123$  and hence has the good quantum numbers  $S_{12} = S_{13} = s$ . (Otherwise it cannot couple with, say,  $S_3 = s$  to give  $S_{123} = 0$ ). Note that a vector  $\Psi$  will belong to different  $\mathcal{B}_T$ ’s if it is already uniquely determined by a proper subset of the quantum numbers corresponding to some coupling scheme  $T_1$ . If  $T_2$  is any other scheme containing the same quantum numbers we have necessarily  $\Psi \in \mathcal{B}_{T_2}$ .

We will apply these considerations to the coupling scheme  $T_1 = (2 \rightarrow 23 \rightarrow 123, 5 \rightarrow 56 \rightarrow 456 \rightarrow 123456)$  and the quantum numbers  $S_{23} = S_{56} = s + 1$ ,  $S_{123} = 1$ ,  $S_{123456} = S = 0$ . Obviously, it follows that  $S_{456}$  must have the value 1 and the vector  $\Psi$  is uniquely determined by these quantum numbers. The same subsystems 23, 56, 123, 123456 also occur in the coupling scheme  $T_2 = (5 \rightarrow 56, 2 \rightarrow 23 \rightarrow 123 \rightarrow 1234 \rightarrow 123456)$ . Hence  $\Psi \in \mathcal{B}_{T_1} \cap \mathcal{B}_{T_2}$  and thus  $\Psi$  must have the quantum number  $S_{1234} = s + 1$ . Analogously,  $S_{1456} = s + 1$ . It follows that  $\Psi$  is an eigenstate of the Heisenberg Hamiltonian

$$\tilde{H}_1 = \left( \tilde{S}^2 - \tilde{S}_{123}^2 - \tilde{S}_{456}^2 \right)$$

$$\begin{aligned}
& - \left( \tilde{S}_{1234}^2 - \tilde{S}_{123}^2 - \tilde{S}_4^2 \right) - \left( \tilde{S}_{1456}^2 - \tilde{S}_{456}^2 - \tilde{S}_1^2 \right) \\
& = 2(-\tilde{\mathbf{s}}_1 \cdot \tilde{\mathbf{s}}_4 + \tilde{\mathbf{s}}_2 \cdot \tilde{\mathbf{s}}_5 + \tilde{\mathbf{s}}_2 \cdot \tilde{\mathbf{s}}_6 + \tilde{\mathbf{s}}_3 \cdot \tilde{\mathbf{s}}_5 + \tilde{\mathbf{s}}_3 \cdot \tilde{\mathbf{s}}_6)
\end{aligned} \tag{87}$$

with eigenvalue  $E_1 = -4(s+1)$ . If  $\tilde{H}(a)$  denotes the Hamiltonian according to (16), (17) and  $b = 0$ , we conclude that

$$\tilde{H}(a) = \left( \tilde{S}_{123}^2 - 3s(s+1) + \tilde{S}_{456}^2 - 3s(s+1) \right) - a \tilde{H}_1, \tag{88}$$

and hence  $\langle \Psi | \tilde{H}(a) | \Psi \rangle = 4a(s+1) + 4 - 6s(s+1)$ . This equals  $\langle \Phi | \tilde{H}(a) | \Phi \rangle = -6s(s+1)$  for  $a = a_{\text{crit}} = -\frac{1}{s+1}$  which confirms (21). Note that the argument is not completely rigorous, since we could not exclude other competing ground states than  $\Psi$  for arbitrary  $s$ . However, it is in agreement with our numerical data presented above.

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